An Analytical Solution for Estimating Percolation Rate by Fitting Temperature Profiles in the Vadose Zone

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Abstract

We present a simple analytical solution for one dimensional steady heat transfer with convection and conduction through a multi-layer system such as a vadose zone. We assume that each layer is homogeneous and has a constant thermal diffusivity. The mass/heat flow direction is perpendicular to the layers, and the mass flow rate is a constant. The analytical solution presented in this study also assumes constant known temperatures at the two boundaries of the system. Although the analytical solution gives the temperature as a function of a few parameters, we focus on the inverse application to estimate the percolation rate in a vadose zone. Example applications have shown that with reliable field observation data, the solution can be used to determine the percolation rate to high degree of accuracy (e.g., to mm/y). In some other cases the solution may also be helpful in characterizing potential lateral flow along layer divides.

Keywords: One-dimensional; Analytical solution; Vadose zone; Percolation rate.

Introduction

Percolation rate is an important parameter in many field problems. For example, it determines the amount of water that is added to groundwater (also called recharge rate) and thus determines the underlying aquifer's capability in water supply. Where the soil is contaminated along the percolation pathway, the product of concentration in soil water and the percolation rate is the contaminant mass loading rate to groundwater. In nuclear waste disposal, "characterization of recharge rate and matrix porosity are the most important factors in the reduction of uncertainty in travel-time estimates" (Nichols and Freshley, 1993).

Although laboratory studies were conducted to determine this important parameter (e.g., Nimmo et al., 1994), measuring percolation rate is by nature a field problem. In theory, percolation rate is the product of hydraulic conductivity and the hydraulic gradient, which are controlled by the soil texture and the boundary conditions. Estimation of the hydraulic gradient and hydraulic conductivity based on field data has been a common practice for a long time. However, the accuracy of such estimation (especially for unsaturated hydraulic conductivity) can greatly affect the accuracy of the calculated percolation rate. Indirect methods have been developed to estimate the percolation rate. For decades, researchers have been using the chloride-mass balance method to estimate recharge rates (e.g., Allison and Hughes, 1978; Scanlon, 1991 & 1992). The method is simple, inexpensive, and capable to provide reliable results in some cases. However, the assumptions that have formed the basis of the method may limit its application in some other cases (Wood, 1999). Another method takes advantage of temperature difference partially caused by fluid flow. For a one-dimensional problem, if a temperature profile in a single layer is not a straight but curved line, the curvature is usually caused by heat convection through fluid flow. Since the measurements of temperature and soil thermal conductivity are relatively simple and accurate, the estimated percolation rate using a temperature profile is expected to be more reliable.

As a general research topic, heat transfer in porous media has been studied by many researchers in different fields (e.g., Clauser, 1987). Applications of these studies in petroleum engineering can be found in Kutasov (1999). Scanlon (1994), and Scanlon and Milly (1994) conducted Field studies on water flow and heat flux in desert soils. Ren et al. (2000) used a heat pulse technique to determine soil water flux and pore water velocity, where the non-uniform temperature distribution was initiated artificially. Bredehoeft and Papadopulos (1965) used a temperature profile to match a corresponding analytical solution in a single layer, and determined the rate of vertical groundwater movement in an aquifer. Sorey (1971) applied this method to field data from the San Luis valley of Colorado and the Roswell basin of New Mexico. He found that the results "were in good agreement with rates computed from pumping tests and water budget methods" (Sorey, 1971). Very recently, Constantz et al. (2001a and 2001b) presented more studies on using heat as a tracer for estimating groundwater recharge. Since a vadose zone is usually composed of different soil (or rock) layers, for purpose of generality, we derive an analytical solution for a vadose zone with n horizontal layers and show the applications in determining the percolation rate.

Researches on heat transfer in multi-layered porous media can be found in the literature (e.g., McKibbin and O'Sullivan, 1980, 1981; McKibbin and Tyvand, 1982, 1983). In these studies, the multi-layered porous media was a bounded saturated system that was heated from below, and the flow of water (circulation) was caused by the thermal gradient. Here in the current study, we are interested in a multi-layered vadose zone with a gravity-driven mass flux, i.e. the percolation.

Theory

An important parameter for heat transfer is the thermal diffusivity, α (in m^2/s) defined by

$$\alpha = \frac{\lambda}{\rho c} \tag{1}$$

where λ is the thermal conductivity (in W/m/^oK); ρ and c are the density (in kg/m^3) and specific heat capacity (in J/kg/^oK) of water, respectively, and the product of the two is called the heat capacity that is an assumed constant (4.18×10^6 J/ $m^3/^oK$) in this study.

To simplify the problem we make the following assumptions: (1) the percolation is in the vertical direction; (2) the percolation rate is a constant; (3) the thermal conductivity (or diffusivity) is a constant for each layer; (4) the effect of latent heat is negligible; and (5) the temperature profile has reached a steady (or quasi-steady) state.

Among these assumptions, the most important ones are the steady-state percolation and heat transfer that must be validated by an observed steady temperature profile. The assumption of a constant thermal diffusivity in each layer can be a rough approximation. In a homogeneous geologic layer under steady-state percolation, the moisture content varies across the layer. Changes can be large near the layer divides. For a dry vadose zone, however, this variation is unlikely to cause significant change in thermal diffusivity of the geologic layer because water occupies only a small portion of the soil. For a wet vadose zone, the moisture content effect can be large, and we may want to divide the vadose zone into more layers according to a measured thermal diffusivity profile. The effect of latent heat is neglected because we assume a single-phase water flow. In cases where gas flow is relatively significant, the latent heat may have a noticeable impact on temperature profile, and we need to use an appropriate numerical code to solve the problem. All the assumptions lead to potential limitations for the solution in field applications. Nevertheless, they reduce the governing equation into the following simple form:

$$\alpha_i \frac{d^2 T_i}{dz^2} = v \frac{dT_i}{dz} \quad (i = 1, 2, \cdots, n) \tag{2}$$

where z is the vertical coordinate, m; T_i is the temperature at arbitrary point in layer *i*, $^{\circ}$C; v is the Darcy velocity (the percolation rate) of water across all layers, m/s; α_i is the thermal diffusivity of the *i*th-layer, m^2/s. The general solution of (2) is:

$$T_i(z) = C_{i.1} e^{vz/\alpha_i} + C_{i.2} \quad (i = 1, 2, \cdots, n) \tag{3}$$

where $C_{i.1}$ and $C_{i.2}$ are two integral constants.

For convenience, we set the origin at the surface of the top layer (note: not necessarily the land surface) and the z axis positive downward (see Figure 1 for a schematic view of a vadose zone with five layers). If we designate the base of each layer a depth of d_i ($i = 1, 2, \cdots, n$), then the thickness of each layer is simply the difference of its two boundary coordinates, i.e.,

$$b_i = d_i - d_{i-1} \quad (i = 1, 2, \cdots, n) \tag{4}$$

where $d_0 = 0$.

Assuming that temperatures at the top and bottom of the system are two different constants, T_0 and T_B, respectively, we then have the boundary conditions as follows:

$$T_1(0)=T_0; \qquad T_n(d_n)=T_B \tag{5a}$$

$$T_i(d_i)=T_{i+1}(d_i) \quad (i=1,2,\cdots,n-1) \tag{5b}$$

$$\alpha_i\left(\frac{dT_i}{dz}\right)_{z=d_i}=\alpha_{i+1}\left(\frac{dT_{i+1}}{dz}\right)_{z=d_i} \quad (i=1,2,\cdots,n-1) \tag{5c}$$

For a given vadose zone, the condition at the lower boundary usually depends on the percolation rate (Constantz et al., 2003). Thus it is necessary to validate (5a) against field data before applying the analytical solution. If the n solutions given by (3) are substituted into boundary conditions (5a) through (5c) we obtain $2n$ linear algebraic equations. Solving these equations simultaneously, we obtain the integral constants as follows:

$$C_{i.2}=\frac{aT_0-T_B}{a-1} \qquad (i=1,2,\cdots,n) \tag{6a}$$

$$C_{1.1}=\frac{T_B-T_0}{a-1} \tag{6b}$$

$$C_{(i+1).1}=e^{vd_i(1/\alpha_i-1/\alpha_{i+1})}C_{i.1} \quad (i=1,2,\cdots,n-1) \tag{6c}$$

where the parameter, a is introduced for convenience and is defined by

$$a=e^{vd_n/\alpha_{eff}} \tag{7}$$

where d_n represents the total thickness of the n layers, and α_{eff} is the effective thermal diffusivity of the n layers defined by

$$\alpha_{eff}=d_n/\sum_{i=1}^{n}(b_i/\alpha_i) \tag{8}$$

Formula (8) is similar to the calculation of the effective hydraulic conductivity for water flow across a multi-layered saturated porous media.

Sometimes, researchers are interested in the convective and conductive heat fluxes crossing any horizontal plane defined as follows.

$$F_{conv.} = \rho c v T_i \tag{9a}$$

$$F_{cond.} = -\lambda_i \left(\frac{dT_i}{dz} \right) \tag{9b}$$

Substituting (3) into (9a) and (9b) and using (1) we obtain

$$F_{conv.} = \rho c v (C_{i.1} e^{vz/\alpha_i} + C_{i.2}) \tag{10a}$$

$$F_{cond.} = -\rho c v C_{i.1} e^{vz/\alpha_i} \tag{10b}$$

The net heat flux is the sum of the convective and conductive heat fluxes:

$$F_{net} = F_{conv.} + F_{cond.} = \rho c v C_{i.2} \tag{11}$$

Since a is a constant for certain system [see (7) and (8)], $C_{i.2}$ is a constant [see (6a)], too. Thus the calculated net heat flux, F_{net} by (11) is a constant that agrees with the assumption. Although the conductive heat flux is irrelevant to the choice of temperature scale, which is indicated by (10b), (6b) and (6c), the convective heat flux (as well as the net heat flux) is scale-dependent. To have a meaningful convective heat flux value, we shall use the bottom temperature as the reference temperature for a later heat flux calculation.

Results and Applications

Solution Verifications

To verify the analytical solution we may set the number of layer, $n = 1$. It can be shown that the multi-layer solution is reduced to the analytical solution given by Bredehoeft and Papadopulos (1965). The analytical solution is also compared with the TOUGH2 (Pruess, 1991) solution in Figure 2. In simulating the one-dimensional problem using TOUGH2, we used a uniform grid size of 1m and the same thermal data, percolation rate, boundary conditions as those used for the analytical solution. We specified an arbitrary temperature profile for the initial condition and run the program to steady state. In Figure 2 the TOUGH2 solution (the circles) matches the analytical solution (the solid line) very well.

Typical Results

We want to use the analytical solution to show some typical results that can be found in field studies. Considering a two-layer vadose zone, each layer is 5m thick. The thermal conductivity is 2 W/m/^{o}K for the top layer, and 1 W/m/^{o}K for the bottom layer. The temperatures are 5 ^{o}C at the surface, and 15 ^{o}C at the base of the vadose zone. The steady temperature profile is calculated for two assumed percolation rates: one is 10^{-7} m/s, and the other is 5×10^{-7} m/s. Two percolation rates at the same order of magnitude result in a great difference in calculated temperature profiles as shown in Figures 3. The results indicate that the method of temperature profile for determining the percolation rate can be relatively accurate.

Application Example

We take the borehole data collected at Well SD-12 of the Yucca Mountain Site (Bodvarsson et al., 1997) to demonstrate an example of application. The site geological survey has indicated that the vadose zone in the particular area is composed of five layers. The depths to the base of each layer and the thermal conductivities for each layer are given in Table 1. A set of observed temperatures at different depths in this well is given in Table 2, including the two temperatures at the top and bottom boundaries. To estimate the percolation rate, v by curve fitting, we first establish a criterion for "best-fit" situation. Here we use the method of root-mean-square (RMS) defined by

$$RMS = \sqrt{\frac{\sum_{j=1}^{m}(T_{cal}^{j} - T_{obv}^{j})^2}{m}} \qquad (12)$$

where m is the number of data points, and inside the parenthesis is the difference of the calculated and observed temperatures at the *j*th level. We are searching for a percolation rate, v such that the corresponding RMS is a minimum. For any given percolation rate, the temperatures at the 16 observation points are calculated using the analytical solution. The corresponding RMS is then calculated using (12). Varying v in a certain range, we obtain a set of RMS values, and a RMS vs. v curve is plotted in Figure 4. Among these calculations, $v =$ 15 mm/y gives the smallest RMS. In Figure 5, four calculated temperature profiles are compared with the observation data, which indicates that the profile corresponding to a percolation rate of $v =$ 15 mm/y gives the best fit to the observation data. The heat flux profiles for the best-fit case are shown in Figure 6. The circles represent the convective heat flux along depth, the triangles represent the conductive heat flux along depth, and the dashed line is the sum of the two fluxes , the net (or total) heat flux. In this case the conductive heat flux at the base of the vadose zone is about -0.047 $J/m^2/s$. The negative sign indicates an upward heat flux.

Effect of Thermal Conductivity

In the inverse application of the solution, temperatures, depths, and thermal conductivities (or diffusivities) are the input data. Among them, temperatures and depths are usually measured at each borehole. The thermal conductivities for the layers may not be available at a borehole to borehole basis. If the thermal data from other boreholes are used in the calculation, one may want to know the impact on the results. In general, the estimated percolation rate increases with the increase of thermal conductivity. In the simplest case where thermal conductivities for all layers are overestimated (or underestimated) by the same percentage, *p*% the estimated percolation rate will also be overestimated (or underestimated) by *p*%. This can be found by evaluation of the governing equation, (2) or the solution (3), and (6) through (8). In practical applications, however, it is not difficult to determine the thermal conductivity for each layer at the observation well fairly accurately. Therefore, the effect of thermal conductivity should not be a concern.

Effect of Lateral Flow

One important assumption that has been made for deriving the analytical solution is a constant flow rate across all layers. What will happen if the flow rate is not a constant but has a reduction at certain depth due to lateral flow? In the following hypothetical example, we want to show that the analytical solution may be able to detect and calculate such a lateral flow that is very useful information in a vadose zone study. We use the same two-layer soils that are used in Figure 3 for the demonstration. This time we assume that there is a very thin layer of clay (we neglect the small thickness of the clay layer for convenience) that cause part of the percolation water go laterally. The "observed" temperature data is shown as triangles in Figures 7a and 7b. In Figure 7a, we applied the solution to the two-layer system and used a single percolation rate to fit the data. It was difficult to fit all data as a whole. In other words, when the fit was good in the top layer, the fit was bad in the bottom layer, and vise versa. The solid curve in Figure 7a is the calculated temperature profile using a percolation rate of 7.5×10^{-8} m/s. Since there is a temperature data at the depth of 5m, we then applied the solution for a single layer and conducted the fitting in each layer independently. In Figure 7b the fitting was obtained using a percolation rate of 10^{-7} m/s in the top layer and a percolation rate of 5×10^{-8} m/s in the bottom layer. The difference of the two percolation rates, 5×10^{-8} m/s is the rate loss due to lateral flow. In this case, half of the percolation from the top layer goes laterally.

Summary and Conclusions

In addition to its capability of verifying numerical code, the analytical solution presented in this study provides an alternative tool for determining the percolation rate to groundwater. The analytical solution can be applied starting from either the land surface or any depth in the subsurface. The division of the layers should be decided based on field thermal conductivity data incorporating with apparent deflection points on the observed temperature profile. The solution is applicable as long as the observed temperature profile does not change much for a period of time, and the calculated percolation rate is valid only for that period of time. For shallow soils where temperatures are very sensitive to the rapid changes of surface temperatures, a steady state may never be reached and a transient solution is needed. The solution was derived based on the assumption of homogeneity for each layer. Thus any heterogeneity such as fractures in a layer will cause the solution inapplicable to that layer. The solution assumes a single-phase water flow and thus neglects the effect of latent heat. When gas flow is relatively significant, the effect of latent heat can be important, and users need to find an appropriate numerical code to solve the problem. In summary, it is always necessary to validate the assumptions before applying the solution.

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Table 1. Layer geometry and thermal conductivity at Well SD-12

i	λ_i (W/m·K)	d_i (m)
1	1.89	53.21
2	0.66	73.09
3	1.70	183.49
4	2.29	373.99
5	1.20	411.17

Table 2. Observed temperatures at Well SD-12

z (m)	0	19.20	40.54	52.12	67.05	82.89	104.24	146.30
T (^{o}C)	17.62	17.82	18.12	18.35	18.85	19.40	19.93	20.97

z (m)	183.49	212.14	231.95	260.3	297.79	360.88	382.52	411.17
T (^{o}C)	21.79	22.21	22.60	23.11	23.78	24.76	25.32	26.48

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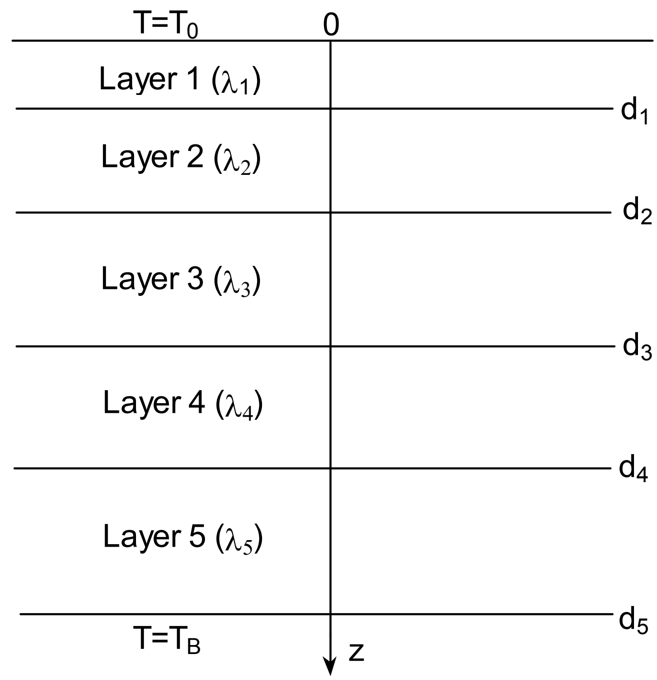

Fig. 1 Schematic section of a five-layer vadose zone

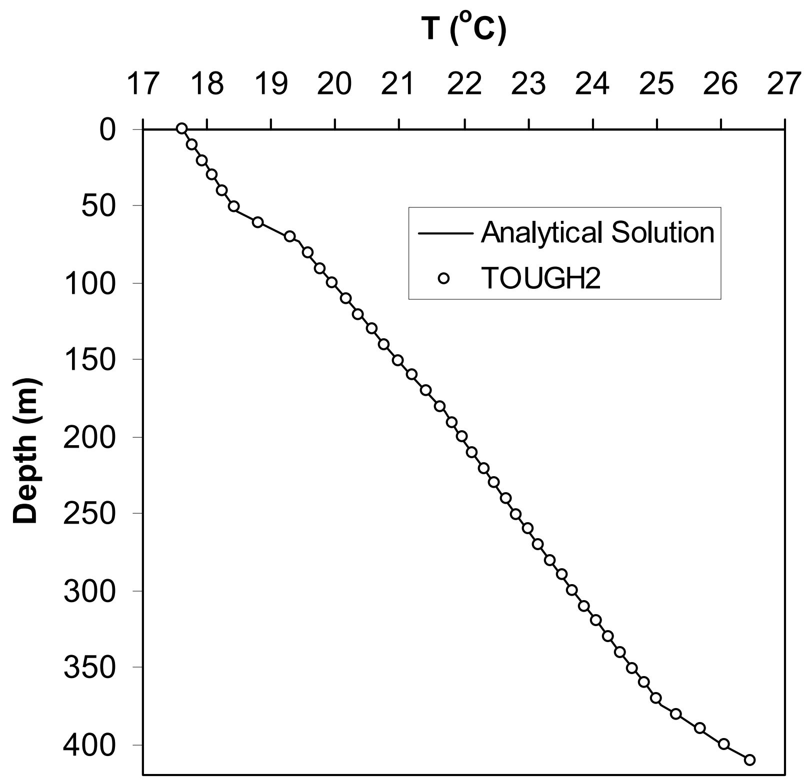

Fig. 2 Comparison of the analytical solution with TOUGH2 solution

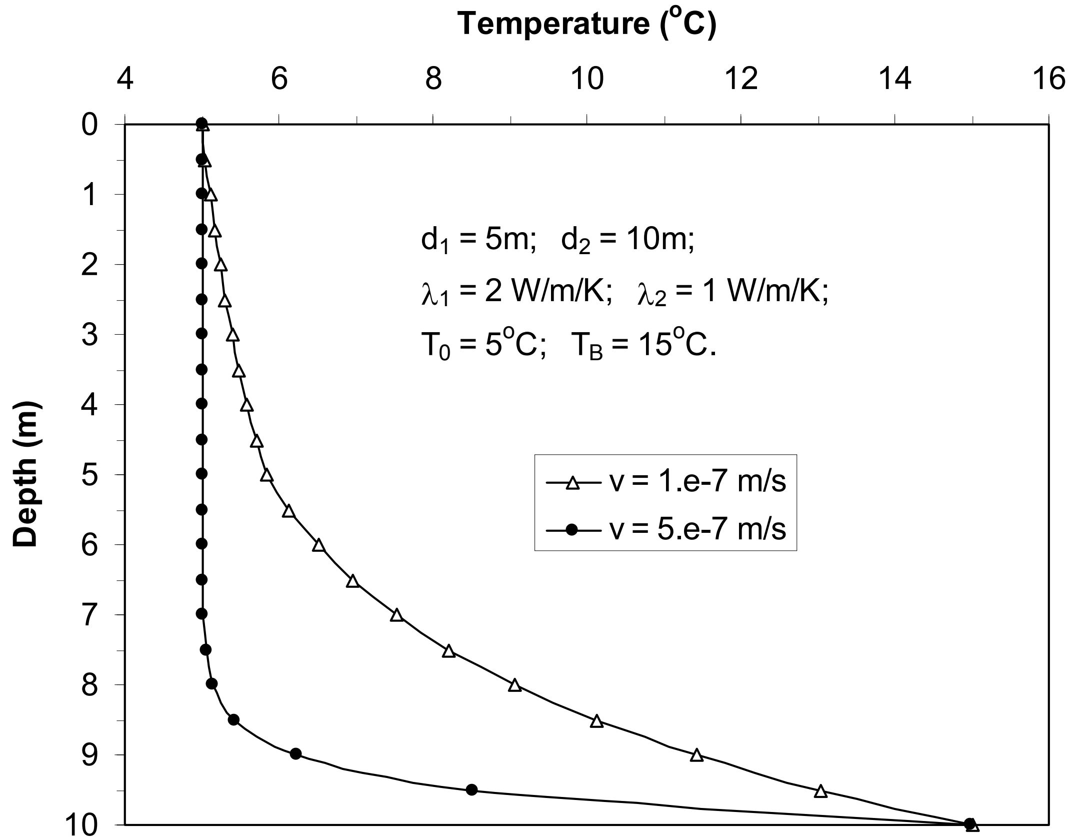

Fig. 3 Example temperature profiles due to percolation in two-layer soils

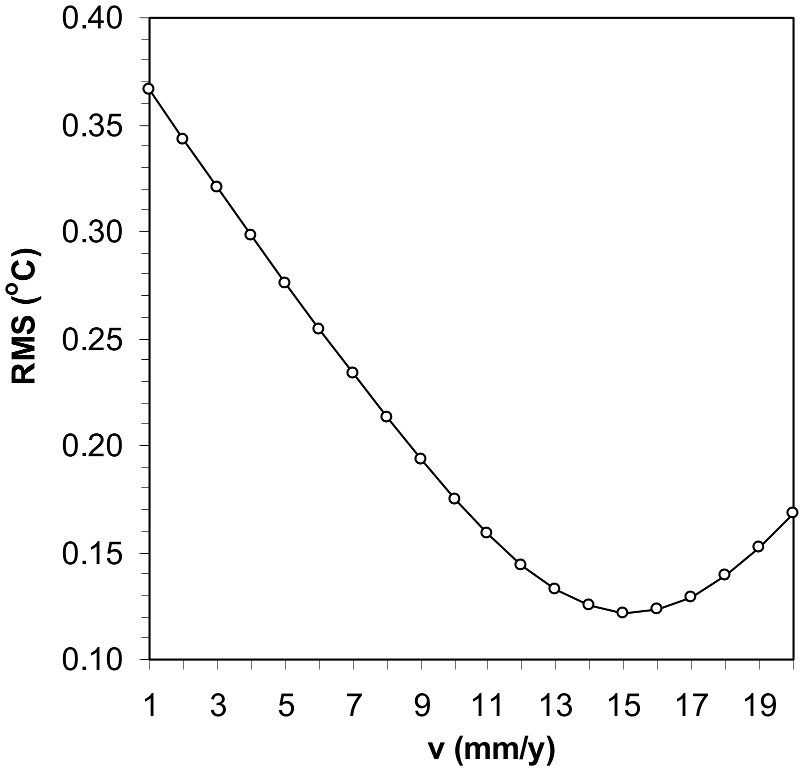

Fig. 4 RMS vs. percolation rate, *v* at Well SD-12

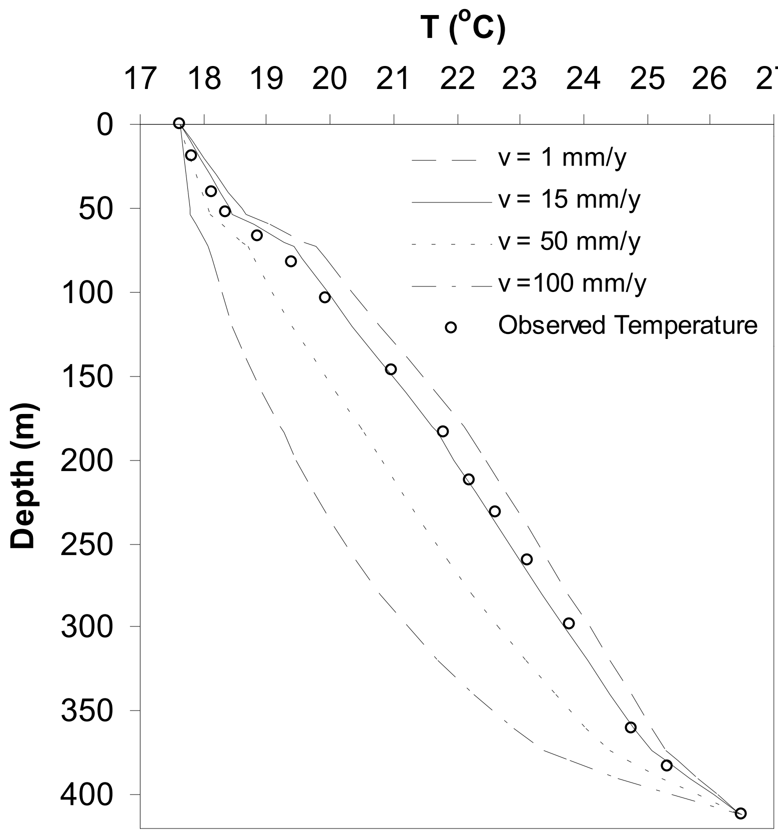

Fig. 5 Comparison of the calculated and observed temperature profiles at Well SD-12

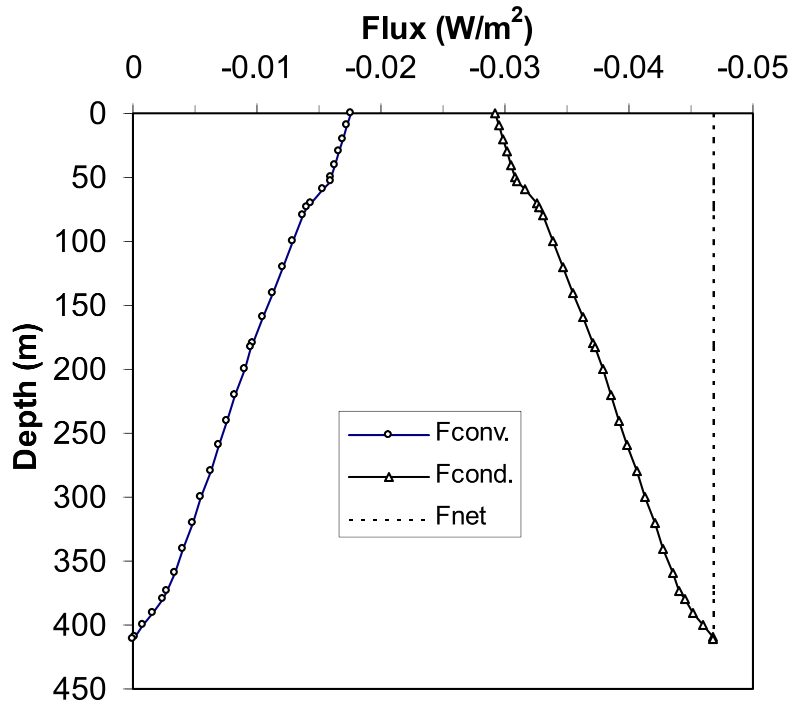

Fig. 6 The heat fluxes for the case of v = 15 mm/y at Well SD-12

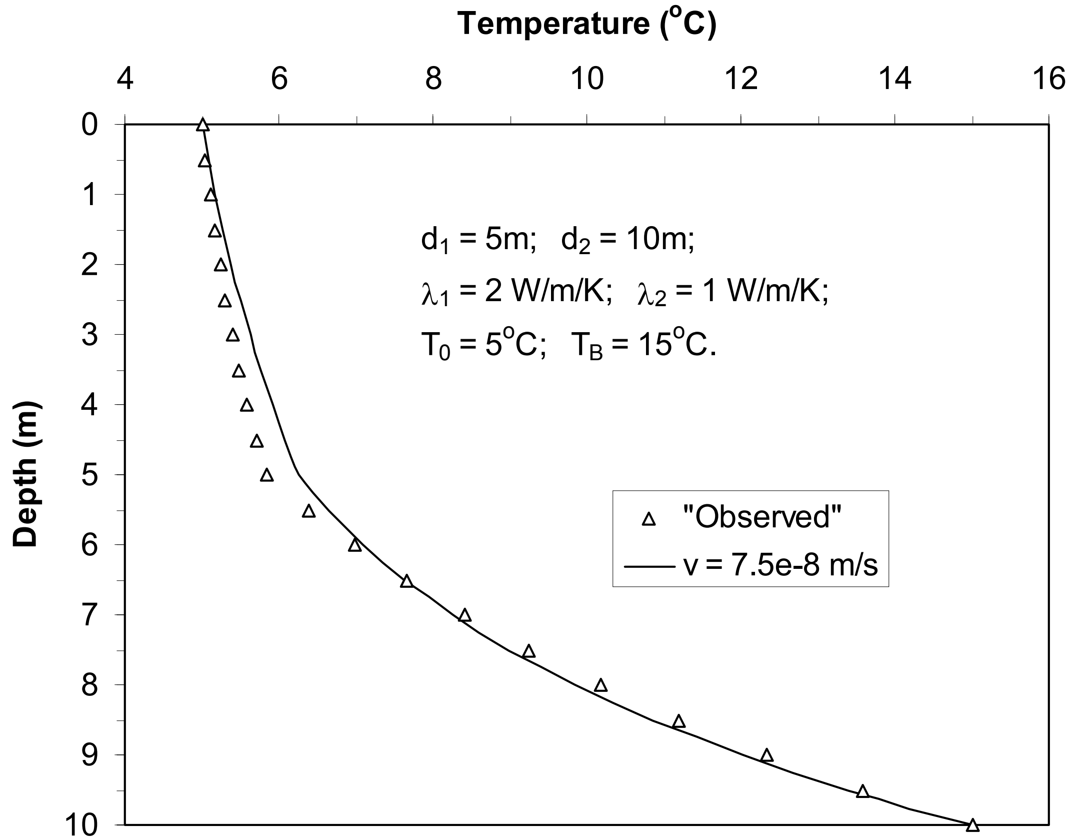

Fig. 7a Fitting temperature data using a single percolation rate in two-layer soils

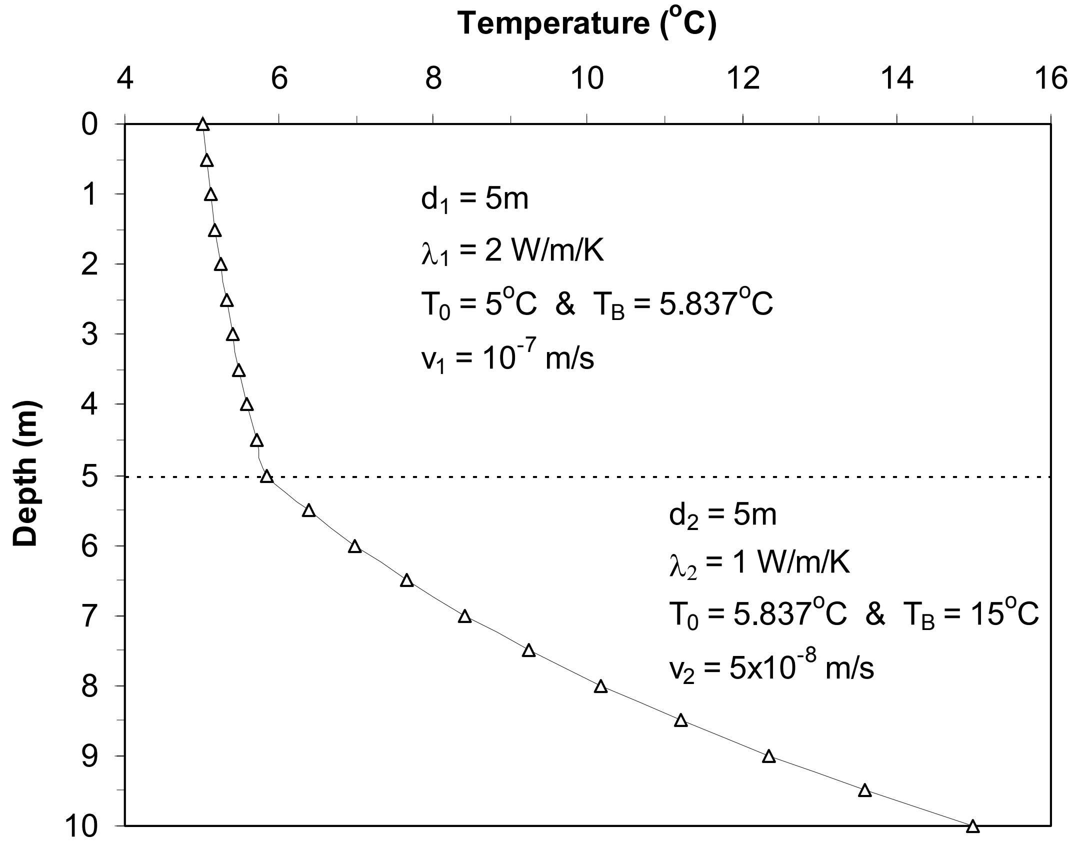

Fig. 7b Fitting temperature data using two percolation rates in two-layer soils